

2,2-Bis(bromomethyl)-1,3-propanediol
3296-90-0 | DTXSID9020164

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.35

Global applicability domain: Inside

Local applicability domain index: 5.72e-01

Confidence level: 6.95e-01

Nearest Neighbors from the Training Set

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35

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2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00

Predicted: 1.47

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4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23